# CONVERGENT PERTURBATION EXPANSION FOR THE ANHARMONIC OSCILLATOR

C.K. AU [1], G.W. ROGERS and Y. AHARONOV [2]
*Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208, USA*

Received 9 December 1982
Revised manuscript received 11 March 1983

We study the ground state as well as the first three excited states of the anharmonic oscillator with anharmonicity $\lambda x^4$ for a range of $\lambda = (0, 10)$ with the first-order logarithmic perturbation iteration method (FOLPIM). This leads to convergent results. The initial choice of the wave function seems only to affect the rate of convergence in the case of the ground state but may critically affect the convergence for the excited states. For large values of $\lambda$, convergence is best obtained by choosing the asymptotic solution as the initial "unperturbed" wave function.

The perturbative solution of the ground state of the anharmonic oscillator has been extensively studied [1–23]. In the typical problem where the anharmonicity is $\lambda x^4$, the energy corrections have been calculated by Bender and Wu to 150 orders [4]. The asymptotic form for the energy correction as a function of the order of the perturbation parameter $\lambda$ has also been given [4]. The resultant series is well known to be divergent. Both the Padé approximation and the Borel summation method have been used to recover finite results for the energy correction [13,14,18]. In the past few years, there has been a lot of renewed interest in the logarithmic perturbation theory which essentially consists of transforming the Schrödinger equation to Ricatti form by taking the logarithm of the wave function [8–11,24–28]. For the case of the ground state where the wave function does not contain any zero, the logarithm is regular. For excited states where the wave functions have nodes, the zeros must be factored out before the logartihm is taken of the envelope of the wave function [24].

The logarithmic perturbation expansion has been used to restudy the $\lambda x^4$ anharmonic oscillator to 72nd order. We have calculated the corrections to the energy and the logarithmic derivative of the wave function. The $i$th-order correction to the logarithmic derivative of the wave function is a polynomial of degree $2i + 1$, consisting of odd powers only. We have compared our results for the energy correction to those of Bender and Wu [4]. Up to the *45th* order, our results are identical to theirs to *12* significant figures. Slight discrepancies slowly accumulate as the order of the perturbation is increased until at the *72nd* order. the agreement with the results of Bender and Wu is only to *3* significant figures. We have run our program in both double- and quadruple-precision versions with exact agreement up to 12 places at 72nd order. We do not understand the reasons for the difference between our results and those of Bender and Wu. Nevertheless, our results confirm their asymptotic form. Hence the straightforward logarithmic perturbation method will not improve the convergence of the perturbation series.

A variant of the logarithmic perturbation method which uses the asymptotic solution to the total potential, $V = V_0 + \lambda V_1$, as an input has been suggested [9, 10, 28]. This input wave function $\psi_0^{\mathrm{I}}$ in logarithmic form is an exact ground-state solution for a potential $V_0^{\mathrm{I}}$. Thus $V_1^{\mathrm{I}} \equiv V - V_0^{\mathrm{I}}$ can be treated as a perturbation to a problem for which we have a solution. This leaves us a "perturbation" which is nonzero, and, may even be large but finite, over a finite measure, com-

[1] On sabbatical leave at the Institute for Theoretical Physics, Santa Barbara, while part of this work was done.
[2] Also at the Physics Department, Tel Aviv University, Ramat Aviv, Israel.

0 031-9163/83/0000–0000/$ 03.00 

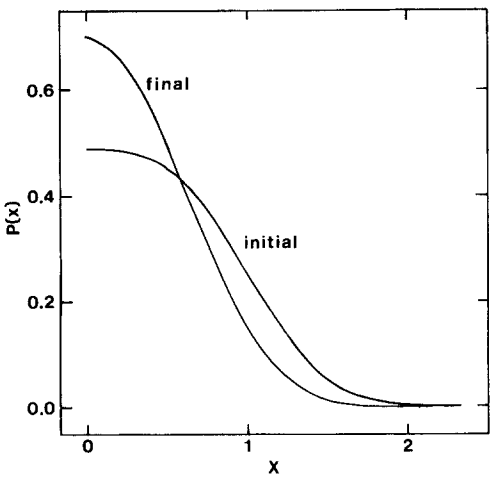


Fig. 1. The probability density $P(x) = \psi^2(x)$ for the initial (asymptotic) and final ground-state wave functions with $\lambda = \frac{1}{2}$.

pared to the original $\lambda x^4$ perturbation which becomes arbitrarily large over a nonfinite measure. Thus one can expect this modification to improve convergence.

In particular, this works well with the first-order-logarithmic perturbation iteration method (FOLPIM) [25]. Here we use the same notations: $G = -\ln \psi$ and $g = G'$, where the prime indicates a derivative with respect to its argument. Using the asymptotic solution

$$g_A(x) = \sqrt{2\lambda}x^2 = g_0^0 , \tag{1}$$

as an input to the Ricatti equation

$$g'(x) - g^2(x) = 2(E - \tfrac{1}{2}x^2 - \lambda x^4) , \tag{2}$$

in *four* iterations, we obtain agreement with the values of Biswas et al. [‡1] to 4 significant figures for $\lambda$ between 0 and 10.0. The result is shown for $\lambda = 0.5$ in fig. 1. The correction to the energy for $\lambda = 10.0$ in each step of the iteration process is displayed in table 1.

For the case of the ground state, FOLPIM will yield a convergent result even *without* using the asymptotic solution as input. As noted in the original paper where FOLPIM was developed [25] (the notation here is the same as in this reference) the energy of the system at the end of the $N$th iteration is ($N \geqslant 2$):

$$E_0^N = E_0^{N-1} + E_1^{N-1} , \tag{3}$$

where

$$E_1^{N-1} = \langle \psi_0^{N-1} | V_1^{N-1} | \psi_0^{N-1} \rangle , \tag{4}$$

and

$$V_1^{N-1} = -\tfrac{1}{2}(g_1^{N-1})^2(\lambda^2)^{N-1} . \tag{5}$$

Thus $E_1^{N-1}$ is negative definite and the FOLPIM scheme yields a monotonically decreasing sequence for the energy eigenvalue: $E_0^N < E_0^{N-1}$. Since

$$E_0^N = \langle \psi_0^{N-1} | H | \psi_0^{N-1} \rangle , \tag{6}$$

where $H$ is the total hamiltonian and $\psi_0^{N-1}$ is the properly normalized eigenfunction of $H_0^{N-1}$ with energy eigenvalue $E_0^{N-1}$, $E_0^N$ is an upper bound to the

[‡1] The reader may refer to ref. [6] for the eigenvalues as a function of the parameter $\lambda$.

Table 1
Convergence of the energy expectation value for the ground state of the $\lambda x^4$ anharmonic oscillator ($\lambda = 10$).

| Iteration step | Asymptotic solution as input | | Harm. osc. ground-state wave function as input | |
|---|---|---|---|---|
| | correction to the energy | energy expectation value [a] | correction to the energy | energy expectation value |
| 0 | 0 | 0 | 0 | $\frac{1}{2}$ |
| 1 | 1.66070 | 1.66070 | 7.500 | 8.000 |
| 2 | $-1.54813 \times 10^{-1}$ | 1.50589 | −3.742 | 4.258 |
| 3 | $-9.21485 \times 10^{-4}$ | 1.50497 | −1.796 | 2.462 |
| 4 | $-9.60965 \times 10^{-9}$ | 1.50497 | −0.707 | 1.755 |
| 5 | $-1.25208 \times 10^{-17}$ | 1.50497 | −0.134 | 1.621 |

[a] Energy expectation value according to Biswas et al. [6] = 1.50497.

true energy. Therefore FOLPIM yields a decreasing sequence of upper bounds. If the system has a true ground state, then this sequence is bounded from below by the true energy. A monotonic decreasing sequence bounded from below will converge to the correct value [29].

We have indeed applied FOLPIM to the anharmonic-oscillator problem with the ordinary harmonic-oscillator ground-state wave function as the input unperturbed wave function. In contrast to the standard perturbation expansions which diverge, both the wave function and energy converge. For $\lambda = \frac{1}{2}$, corrections on the fifth iteration are five orders of magnitude less than those obtained in the first iteration and are already in agreement with the published values of Biswas et al. [6]. We illustrate the convergence of the sequence $\{V_1^N\}$ in fig. 2 for $\lambda = \frac{1}{2}$. For large $\lambda$, say $\lambda = 10$, we encounter computational difficulties because of the simultaneous appearance of very large and very small numbers. It is thus much harder to achieve good accuracy due to difficulties arising from numerical approximations. Nevertheless, the iteration process does seem to yield a decreasing sequence for the energy expectation value. For the purpose of comparing how the initial choice of the wave function affects the rate of convergence in the case of the ground state, we also show in table 1 the corrections to the energy and the energy expectation value in each step of the iteration process, when the harmonic-oscillator ground-state wave function is used as the input.

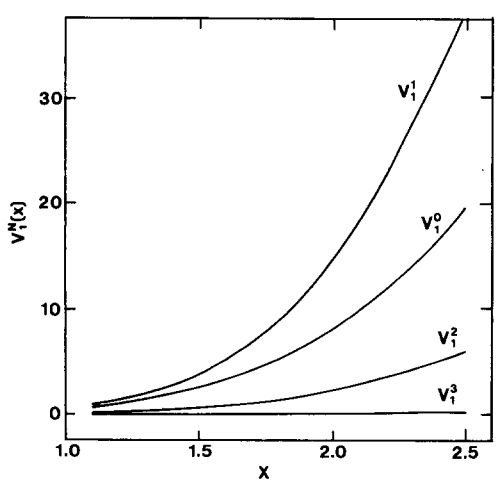


Fig. 2. The effective perturbation potential $V_1^N(x)$ for the first three iterations with $\lambda = \frac{1}{2}$, with the harmonic-oscillator ground-state wave function as the initial input FOLPIM.

Finally, we would like to report on the application of FOLPIM to the excited states of the anharmonic oscillator, where the wave functions have zeros:

$$\psi_{n,\mathrm{ex}}(x) = \prod_{i=1}^{n} (x - \alpha_i) \mathrm{e}^{-G(x)} . \tag{7}$$

The Ricatti equation becomes

$$g^2 - g' - 2g \sum_{i=1}^{n} 1/(x - \alpha_i) + 2 \sum_{i=1}^{n} \sum_{j>i}^{n} 1/(x - \alpha_i)(x - \alpha_j) = 2(V - E) . \tag{8}$$

Since $g \equiv G'$ is regular, we have, for a nonsingular potential $V$:

$$g(\alpha_i) = \sum_{j \neq i} 1/(\alpha_i - \alpha_j) . \tag{9}$$

Eq. (9) serves as a very important constraint relation on the nodes and logarithmic derivative of the wave function envelope.

To generate the solution for the $n$th excited state, we start with the ground-state solution $g_{\mathrm{gr}}$ and $E_{\mathrm{gr}}$, which satisfies:

$$g_{\mathrm{gr}}^2 - g_{\mathrm{gr}}' = 2(V - E_{\mathrm{gr}}) . \tag{10}$$

The $n$th excited state has $n$ nodes in the wave function. The input wave function in this case is chosen to be

$$\psi_0^0 = \psi_{n,\mathrm{ex}}^{\mathrm{input}} = \prod_i (x - \alpha_i^{(0)}) \exp(-G_{\mathrm{gr}} + C) , \tag{11}$$

where $C$ is a suitable normalization constant and the nodes $\{\alpha_i^{(0)}\}$ are chosen in accordance with the constraint equation (9) as well as symmetry considerations. The choice of the envelope to be that of the ground-state solution ensures the correct asymptotic behavior. The wave function expressed in eq. (11) is a solution to the Ricatti equation (8) for a potential $(V - \Delta V)$. Since the nodes are chosen in accordance with the constraint equation (9), $\Delta V$ is regular and hence we can apply FOLPIM to $\Delta V$. For $\lambda = 0.5$, by using FOLPIM, five iterations lead to results that agree with those of Biswas et al. [6] to five significant figures for the first two excited states and to three places for the

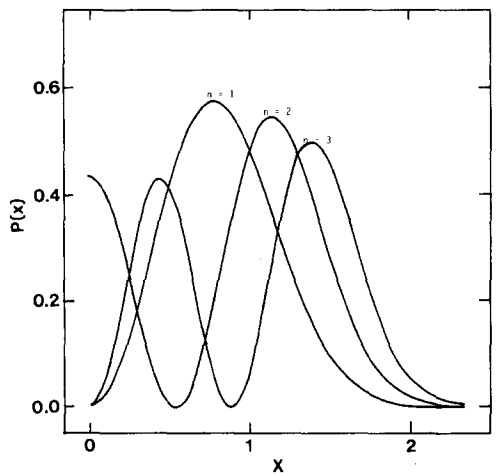


Fig. 3. The FOLPIM-generated probability density $P(x) = \psi_n^2(x)$ for the first three excited states with $\lambda = \frac{1}{2}$.

third excited state. For smaller values of λ, convergence is even faster. For larger λ, in the range λ = (0,10) we examined, this FOLPIM with the asymptotic solution as input again proves to work very well. For all three states considered, for λ = (0, 10), the corrections obtained in the sixth iteration are at least 9 orders of magnitude less than those in the first iteration. We illustrate the solutions for the wave functions for λ = 0.5 in fig. 3. We also illustrate the convergence of the energy expectation value in FOLPIM and the adjustment in the positions of the nodes in each step of the iteration process for λ = 10 for the first, second and third excited states in tables 2, 3, and 4. For comparison purposes, we also list the energy expectation value obtained by Biswas et al. [6]. We notice excellent agreement between our results and those of Biswas et al. [6] for the ground and the first excited states. In all cases, in the numerical integration, we encounter the simultaneous appearance of large and small numbers and we have to introduce numerical cutoffs in the numerical integration. Such cutoffs probably account for the disagreement between our result and that of Biswas et al. for the second and third excited states. Unfortunately, we do not have a fair estimate of the errors due to our cutoff.

Lastly, we would like to comment on the question of convergence in the two FOLPIM methods considered. For the ground state it appears that (numerical problems aside) the FOLPIM method leads to convergent and correct results for either kind of trial wave function considered. For the asymptotic trial wave function, convergence is quite rapid for all λ between 0 and 10. For the harmonic-oscillator trial wave function, convergence is slowed as λ increases. Nevertheless, convergence is not in question, rather the exact result becomes more dependent on the numerical routine used and hence high accuracy becomes harder to obtain as λ is increased.

The situation with the excited states is more complicated. In contrast to the ground state, $E_1^N$ for $N > 1$ is not negative definite as can be seen in tables 3 and 4 for the second and third excited states. If the trial wave function is "close" enough to the exact solution there seems to be no problem with convergence. If the trial wave function differs too much, convergence is definitely difficult to attain for higher excited states. In fact, for some (dependent on the trial wave function), the nodes may be shifted past the classical turning points or inward past the origin. This

Table 2
Convergence of the energy expectation value and the adjustment in the nodal position for the first excited state of the $\lambda x^4$ anharmonic oscillator (λ = 10).

| Iteration step | Correction to the energy | Energy expectation value [a] | Correction to nodal position | Nodal position |
|---|---|---|---|---|
| 0 | 0 | 1.50497 | 0 | 0 |
| 1 | 3.84550 | 5.35047 | 0 | 0 |
| 2 | $-2.88495 \times 10^{-2}$ | 5.32162 | 0 | 0 |
| 3 | $-1.64981 \times 10^{-5}$ | 5.32161 | 0 | 0 |
| 4 | $-8.60388 \times 10^{-13}$ | 5.32161 | 0 | 0 |

[a] Energy expectation value according to Biswas et al. [6] = 5.32161. The zeroth-order energy is adjusted to be the energy of the ground state.

Table 3
Convergence of the energy expectation value and the adjustment in the nodal position for the second excited state of the $\lambda x^4$ anharmonic oscillator ($\lambda = 10$).

| Iteration step | Correction to the energy | Energy expectation value [a] | Correction to nodal position | Nodal position [b] |
|---|---|---|---|---|
| 0 | 0 | 1.50497 | 0 | 0.384 |
| 1 | 8.891 | 10.396 | −0.0462 | 0.338 |
| 2 | $-6.537 \times 10^{-2}$ | 10.330 | $0.728 \times 10^{-2}$ | 0.345 |
| 3 | $+5.7818 \times 10^{-3}$ | 10.336 | $0.581 \times 10^{-3}$ | 0.346 |
| 4 | $+2.8459 \times 10^{-4}$ | 10.336 | $0.814 \times 10^{-5}$ | 0.346 |
| 5 | $-2.599 \times 10^{-8}$ | 10.336 | $0.355 \times 10^{-8}$ | 0.346 |
| 6 | $+1.4580 \times 10^{-14}$ | 10.336 | $0.265 \times 10^{-15}$ | 0.346 |

[a] Energy expectation value according to Biswas et al. [6] = 10.3471. The zeroth-order energy is adjusted to be that of the ground-state energy.
[b] The nodes occur symmetrically with respect to the origin.

Table 4
Convergence of the energy expectation value and the adjustment in the nodal position for the third excited state of the $\lambda x^4$ anharmonic oscillator ($\lambda = 10$).

| Iteration step | Correction to the energy | Energy expectation value [a] | Correction to nodal position | Nodal position [b] |
|---|---|---|---|---|
| 0 | 0 | 1.50497 | 0 | 0.617 |
| 1 | 14.702 | 16.207 | −0.6999 | 0.547 |
| 2 | $-8.525 \times 10^{-2}$ | 16.122 | $+0.838 \times 10^{-2}$ | 0.555 |
| 3 | $+1.303 \times 10^{-2}$ | 16.135 | $0.106 \times 10^{-2}$ | 0.557 |
| 4 | $+1.030 \times 10^{-3}$ | 16.136 | $0.366 \times 10^{-4}$ | 0.557 |
| 5 | $+9.414 \times 10^{-7}$ | 16.136 | $0.460 \times 10^{-7}$ | 0.557 |
| 6 | $+1.789 \times 10^{-12}$ | 16.136 | $0.667 \times 10^{-13}$ | 0.557 |

[a] Energy expectation value according to Biswas et al. [6] = 16.090. The zeroth-order energy is adjusted to be that of the ground-state energy.
[b] The nodes occur symmetrically with respect to the origin in addition to the one located at the origin.

situation certainly creates problems in our algorithm. In practice, convergence alsways fails before these values of $\lambda$ are reached. In conclusion, for the excited states the authors can only present the rule of thumb that, as long as the first-order correction to the nodes does not shift them more than a small fraction of the distance between adjacent nodes, our method would probably lead to convergent results. Hence one does rely on the initial choice of the trial wave function. However, we seem to have a "guideline" here, though not a rule. One can hopefully solve the ground-state problem quite accurately with our method. The excited-state trial wave function is chosen with this ground-state envelope and is assigned initial trial nodal positions in accordance with eq. (9). Luckily, this last step is an algebraic process. We would like to add that for large $\lambda$, the $\lambda x^4$ term is dominant. By doing perturbation theory on the deviation from asymptotic behavior, we are effectively treating the $x^2$ term, which is lesser, as a perturbation. From this angle, FOLPIM provides a systematic method to improve on the trial wave function.

This work is supported by the National Science Foundation under Grants No. PHY 79-01053 and ISP 80-11451 and by the University of South Carolina

under Grant No. USC-13070-E121. CKA expresses thanks to Professor W. Kohn of the Santa Barbara Institute and to Professor A. Dalgarno of Harvard–Smithsonian Astrophysics Observatory for their hospitality while part of this work was being done.

*References*

[1] T. Banks and C.M. Bender, J. Math. Phys. 13 (1972) 1320.
[2] C.M. Bender, J. Math. Phys. 11 (1970) 796.
[3] C.M. Bender and T.T. Wu, Phys. Rev. Lett. 27 (1971) 461.
[4] C.M. Bender and T.T. Wu, Phys. Rev. 184 (1969) 1231; Phys. Rev. D7 (1973) 1620.
[5] S.N. Biswas, K. Datta, R.P. Saxena, P.K. Srivastava and V.S. Varma, Phys. Rev. D4 (1971) 3617.
[6] S.N. Biswas, K. Datta, R.P. Saxena, P.K. Srivastava and V.S. Varma, J. Math. Phys. 14 (1973) 1190.
[7] J.C. Collins and D.E. Soper, Ann. Phys. 112 (1978) 209.
[8] A.D. Dolgov, V.L. Eletskiĭ and V.S. Popov, Sov. Phys. JETP 52 (1980) 861.
[9] A.D. Dolgov and V.S. Popov, Phys. Lett. 79B (1978) 403.
[10] V.L. Eletsky and V.S. Popov, Phys. Lett. 94B (1980) 65.
[11] A.D. Dolgov and V.S. Popov, Sov. Phys. JETP 48 (1978) 1012; Phys. Lett. 86B (1979) 185.
[12] G.P. Flessas and G.S. Anagnostatos, J. Phys. A15 (1982) L437.
[13] S. Graffi, V. Greechi and B. Simon, Phys. Lett. 32B (1970) 631.
[14] S. Graffi and V. Greechi, J. Math. Phys. 19 (1978) 1002.
[15] F.T. Hioe and E.W. Montroll, J. Math. Phys. 16 (1975) 1945.
[16] F.T. Hioe, D. MacMillen and E.W. Montroll, J. Math. Phys. 17 (1976) 1320; Phys. Rep. 43 (1978) 305.
[17] J. Killingbeck, J. Phys. A13 (1980) 49.
[18] J.J. Loeffel, A. Martin, B. Simon and A.S. Wightman, Phys. Lett. 30B (1969) 656.
[19] G. Parisi, Phys. Lett. 69B (1977) 329.
[20] C.E. Reid, Int. J. Quantum Chem. 1 (1967) 521.
[21] C. Schwartz, Ann. Phys. 32 (1965) 277.
[22] B. Simon, Ann. Phys. 58 (1970) 76.
[23] J. Zinn-Justin, Phys. Rep. 70 (1981) 109.
[24] Y. Aharonov and C.K. Au, Phys. Rev. Lett. 42 (1979) 1582.
[25] C.K. Au, Phys. Lett. 77A (1980) 221.
[26] V. Privman, Phys. Rev. A24 (1981) 2362.
[27] V.S. Polikanov, Sov. Phys. JETP 25 (1967) 882.
[28] A.V. Turbiner, Sov. Phys. JETP 52 (1980) 868.
[29] V. Privman, private communication (1981); Technion report PH-81-33 (1981).